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NEWS 15 OCT 27 EPFULL enhanced with additional content  
NEWS 16 NOV 14 CA/CAPLUS - Expanded coverage of German academic research  
  
NEWS EXPRESS JUNE 13 CURRENT WINDOWS VERSION IS V8.0, CURRENT  
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005  
  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 15:31:15 ON 14 NOV 2005

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 15:31:22 ON 14 NOV 2005  
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STRUCTURE FILE UPDATES: 13 NOV 2005 HIGHEST RN 867336-65-0  
DICTIONARY FILE UPDATES: 13 NOV 2005 HIGHEST RN 867336-65-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when  
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```
*****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005. A new display format, IDERL, is now     *
* available and contains the CA role and document type information.  *
*
*****
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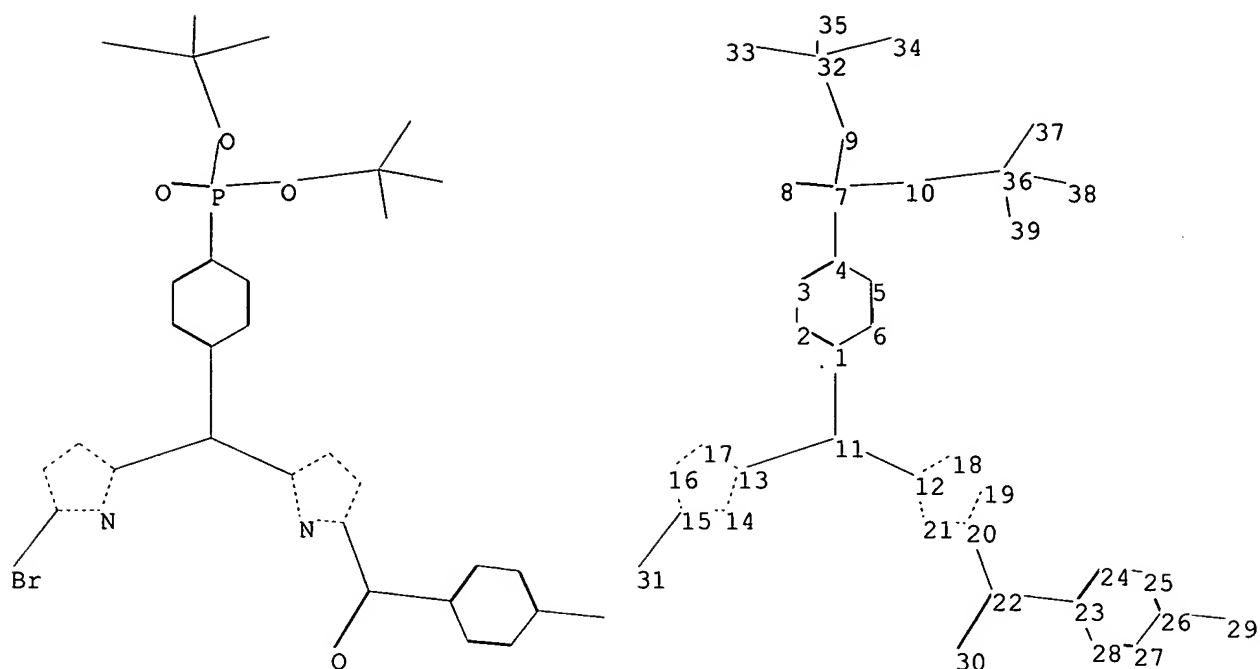
Structure search iteration limits have been increased. See HELP SLIMITS  
for details.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10698255s.str



chain nodes :

7 8 9 10 11 22 29 30 31 32 33 34 35 36 37 38 39

ring nodes :

1 2 3 4 5 6 12 13 14 15 16 17 18 19 20 21 23 24 25 26 27 28

chain bonds :

1-11 4-7 7-8 7-9 7-10 9-32 10-36 11-12 11-13 15-31 20-22 22-23 22-30

26-29 32-33 32-34 32-35 36-37 36-38 36-39

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 12-18 12-21 13-14 13-17 14-15 15-16 16-17

18-19 19-20 20-21 23-24 23-28 24-25 25-26 26-27 27-28

exact/norm bonds :

7-8 7-9 7-10 9-32 10-36 12-18 12-21 13-14 13-17 14-15 15-16 16-17 18-19

19-20 20-21 22-30

exact bonds :

1-11 4-7 11-12 11-13 15-31 20-22 22-23 26-29 32-33 32-34 32-35 36-37

36-38 36-39

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 23-24 23-28 24-25 25-26 26-27 27-28

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS

11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom

20:Atom 21:Atom 22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom

29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS

37:CLASS 38:CLASS 39:CLASS

=> d  
L1 HAS NO ANSWERS  
L1 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> s l1  
SAMPLE SEARCH INITIATED 15:31:42 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 2 TO 124  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full  
FULL SEARCH INITIATED 15:31:45 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 36 TO ITERATE

100.0% PROCESSED 36 ITERATIONS 1 ANSWERS  
SEARCH TIME: 00.00.01

L3 1 SEA SSS FUL L1

=> file caplus  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
ENTRY SESSION  
FULL ESTIMATED COST 161.33 161.54

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FILE COVERS 1907 - 14 Nov 2005 VOL 143 ISS 21  
FILE LAST UPDATED: 13 Nov 2005 (20051113/ED)

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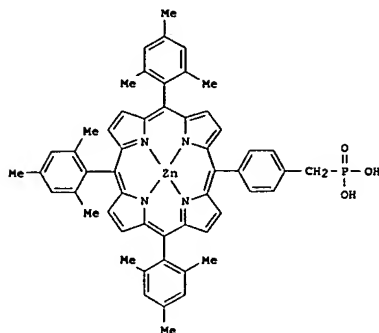
=> s l3  
L4 2 L3

=> d ibib abs hitstr tot

L4 ANSWER 1 OF 2 CAPIUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2005:394876 CAPIUS  
 DOCUMENT NUMBER: 142:440857  
 TITLE: Synthesis of phosphono-substituted porphyrin compounds  
 INVENTOR(S): for attachment to metal oxide surfaces  
 Lindsey, Jonathan S.; Loewe, Robert S.; Muthukumaran, Kannan; Ambrose, Arounaguiry  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 29 pp.  
 CODEN: USXKCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005096465	A1	20050505	US 2003-698255	20031031
PRIORITY APPLN. INFO.:			US 2003-698255	20031031

GI



AB A method is described for making phosphono-substituted dipyrromethane derivs. comprising reacting an aldehyde or acetal having at least one phosphono group with pyrrole to produce a phosphono-substituted dipyrromethane. The phosphono substituent is selected from the group consisting of dialkyl phosphono, diaryl phosphono, and dialkylaryl phosphono. The dipyrromethane is used to prepare phosphono-substituted chlorins and porphyrins which can potentially be attached to metal oxide surfaces. Thus, zinc 5-(4-(phosphonomethyl)phenyl)-10,15,20-

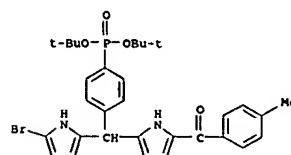
L4 ANSWER 2 OF 2 CAPIUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 2003:965574 CAPIUS  
 DOCUMENT NUMBER: 140:156138  
 TITLE: Porphyrins Bearing Arylphosphonic Acid Tethers for Attachment to Oxide Surfaces  
 AUTHOR(S): Muthukumaran, Kannan; Loewe, Robert S.; Ambrose, Arounaguiry; Tamaru, Shunichi; Li, Qiliang; Mathur, Guru; Bocian, David F.; Misra, Veena; Lindsey, Jonathan S.  
 CORPORATE SOURCE: Departments of Chemistry and Electrical and Computer Engineering, North Carolina State University, Raleigh, NC, 27695-8204, USA  
 SOURCE: Journal of Organic Chemistry (2004), 69(5), 1444-1452  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Synthetic mols. bearing phosphonic acid groups can be readily attached to oxide surfaces. As part of a program in mol.-based information storage, the authors have developed routes for the synthesis of diverse porphyrinic compds. bearing phenylphosphonic acid tethers. The routes enable (1) incorporation of masked phosphonic acid groups in precursors for use in the rational synthesis of porphyrinic compds. and (2) derivatization of porphyrins with masked phosphonic acid groups. The precursors include dipyrromethanes, monoacyldipyrromethanes, and diacyldipyrromethanes. The tert-Bu group was used to mask the dihydroxyphosphoryl substituent. The di-tert-butyloxyporphoryl unit is stable to the range of conditions employed in syntheses of porphyrins and multiporphyrin arrays yet can be deprotected under mild conditions (TMS-Cl/TEA or TMS-Br/TEA in refluxing CHCl3) that do not cause demetalation of Zn or Mg porphyrins. The porphyrinic compds. that were prepared include (1) A3B-, trans-AB2C-, and ABCD-porphyrins that bear a single phenylphosphonic acid group, (2) a trans-A2B2-porphyrin bearing two phenylphosphonic acid groups, (3) a chlorin that bears a single phenylphosphonic acid group, and (4) a porphyrin dyad bearing a single phenylphosphonic acid group. For selected porphyrin-phosphonic acids, the electrochem. characteristics were studied for mols. tethered to SiO2 surfaces grown on doped Si. The voltammetric behavior indicates that the porphyrin-phosphonic acids form robust, elec. well-behaved monolayers on the oxide surface.

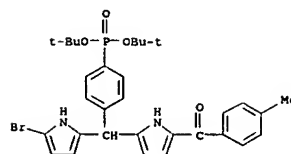
IT 651302-30-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reactant for preparation of magnesium/zinc complexes with porphyrins having arylphosphonic acid tethers)

RN 651302-30-6 CAPIUS  
 CN Phosphonic acid, [4-[(5-bromo-1H-pyrrol-2-yl)[5-(4-methylbenzoyl)-1H-pyrrol-2-yl]methyl]phenyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 2 CAPIUS COPYRIGHT 2005 ACS on STN (Continued)  
 trimesitylporphyrin (I) was prepd. Addnl. methods, intermediates and products are also described.  
 IT 651302-30-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of phosphono-substituted porphyrin compds.)  
 RN 651302-30-6 CAPIUS  
 CN Phosphonic acid, [4-[(5-bromo-1H-pyrrol-2-yl)[5-(4-methylbenzoyl)-1H-pyrrol-2-yl]methyl]phenyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



L4 ANSWER 2 OF 2 CAPIUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

```
=> file reg
COST IN U.S. DOLLARS          SINCE FILE      TOTAL
                                ENTRY      SESSION
FULL ESTIMATED COST          10.33      171.87

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)  SINCE FILE      TOTAL
                                                ENTRY      SESSION
CA SUBSCRIBER PRICE          -1.46      -1.46
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STRUCTURE FILE UPDATES: 13 NOV 2005 HIGHEST RN 867336-65-0  
 DICTIONARY FILE UPDATES: 13 NOV 2005 HIGHEST RN 867336-65-0

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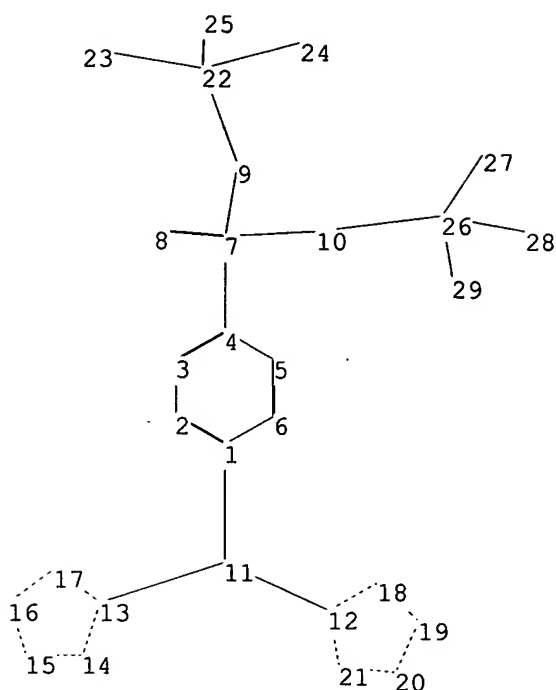
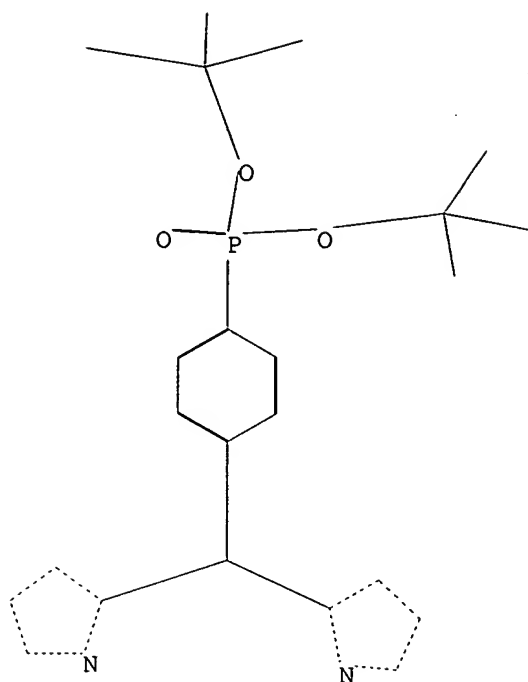
```
*****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
*****
```

Structure search iteration limits have been increased. See HELP SLIMITS  
 for details.

REGISTRY includes numerically searchable data for experimental and  
 predicted properties as well as tags indicating availability of  
 experimental property data in the original document. For information  
 on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

```
=>
Uploading C:\Program Files\Stnexp\Queries\10698255.str
```



chain nodes :

7 8 9 10 11 22 23 24 25 26 27 28 29

ring nodes :

1 2 3 4 5 6 12 13 14 15 16 17 18 19 20 21

chain bonds :

1-11 4-7 7-8 7-9 7-10 9-22 10-26 11-12 11-13 22-23 22-24 22-25 26-27  
26-28 26-29

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 12-18 12-21 13-14 13-17 14-15 15-16 16-17  
18-19 19-20 20-21

exact/norm bonds :

7-8 7-9 7-10 9-22 10-26 12-18 12-21 13-14 13-17 14-15 15-16 16-17 18-19  
19-20 20-21

exact bonds :

1-11 4-7 11-12 11-13 22-23 22-24 22-25 26-27 26-28 26-29

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom  
20:Atom 21:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS  
28:CLASS 29:CLASS

L5 STRUCTURE UPLOADED

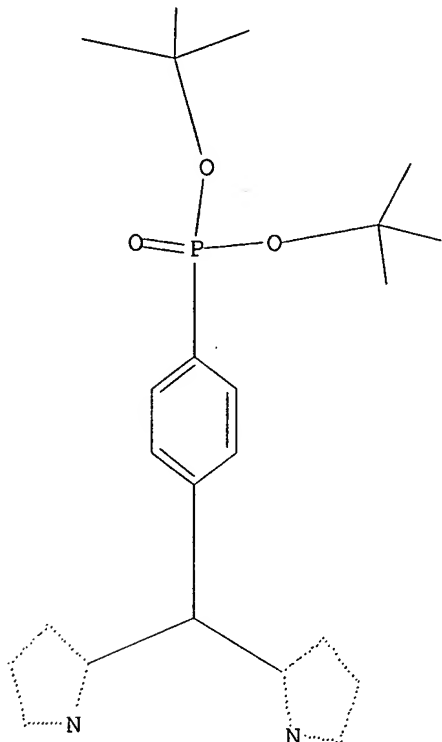
=> dd

DD IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.

For a list of commands available to you in the current file, enter  
"HELP COMMANDS" at an arrow prompt (=>).

=> d  
L5 HAS NO ANSWERS  
L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 15  
SAMPLE SEARCH INITIATED 15:33:01 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE  
  
100.0% PROCESSED 2 ITERATIONS 1 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 2 TO 124  
PROJECTED ANSWERS: 1 TO 80

L6 1 SEA SSS SAM L5

=> s 15 full  
FULL SEARCH INITIATED 15:33:03 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 28 TO ITERATE

100.0% PROCESSED 28 ITERATIONS 4 ANSWERS  
SEARCH TIME: 00.00.01



L7 4 SEA SSS FUL L5

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	161.76	333.63

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-1.46

FILE 'CAPLUS' ENTERED AT 15:33:06 ON 14 NOV 2005  
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FILE COVERS 1907 - 14 Nov 2005 VOL 143 ISS 21  
FILE LAST UPDATED: 13 Nov 2005 (20051113/ED)

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<http://www.cas.org/infopolicy.html>

=> s 17

L8 2 L7

=> d ibib abs hitstr tot

LB ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS ON STN

ACCESSION NUMBER: 2005:394876 CAPLUS

DOCUMENT NUMBER: 142:440857

TITLE: Synthesis of phosphono-substituted porphyrin compounds

INVENTOR(S): for attachment to metal oxide surfaces  
Lindsey, Jonathan S.; Loewe, Robert S.; Muthukumaran, Kannan; Ambrose, Arounaguiry

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 29 pp.

CODEN: USXOXO

DOCUMENT TYPE: Patent

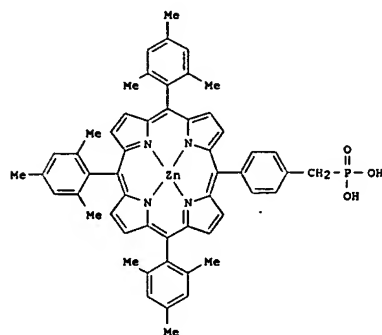
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005096465	A1	20050505	US 2003-698255	20031031
PRIORITY APPLN. INFO.:			US 2003-698255	20031031

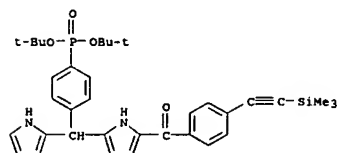
GI



I

AB A method is described for making phosphono-substituted dipyrromethane deriva. comprising reacting an aldehyde or acetal having at least one phosphono group with pyrrole to produce a phosphono-substituted dipyrromethane. The phosphono substituent is selected from the group consisting of dialkyl phosphono, diaryl phosphono, and dialkylaryl phosphono. The dipyrromethane is used to prepare phosphono-substituted chlorins and porphyrins which can potentially be attached to metal oxide surfaces. Thus, zinc 5-[(4-(phosphonomethyl)phenyl)-10,15,20-

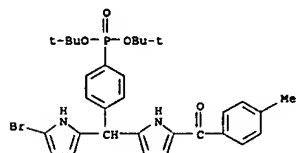
LB ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS ON STN (Continued)



IT 651302-30-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of phosphono-substituted porphyrin compds.)

RN 651302-30-6 CAPLUS  
CN Phosphonic acid, [4-[(5-bromo-1H-pyrrol-2-yl)]-5-(4-methylbenzoyl)-1H-pyrrol-2-yl]methylphenyl-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

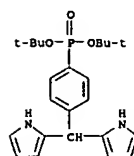
INDEX



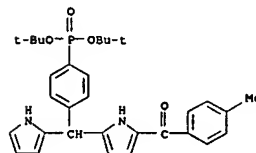
LB ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS ON STN (Continued)  
trimesitylporphyrin (I) was prepd. Addnl. methods, intermediates and products are also described.

IT 651301-78-9P 651301-87-0P 651301-88-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of phosphono-substituted porphyrin compds.)

RN 651301-78-9 CAPLUS  
CN Phosphonic acid, [4-(di-1H-pyrrol-2-ylmethyl)phenyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



RN 651301-87-0 CAPLUS  
CN Phosphonic acid, [4-[[5-(4-methylbenzoyl)-1H-pyrrol-2-yl]-1H-pyrrol-2-ylmethyl]phenyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



RN 651301-88-1 CAPLUS  
CN Phosphonic acid, [4-[[5-(4-methylbenzoyl)-1H-pyrrol-2-yl]-1H-pyrrol-2-ylmethyl]phenyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

LB ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS ON STN

ACCESSION NUMBER: 2003:965574 CAPLUS

DOCUMENT NUMBER: 140:156138

TITLE: Porphyrins Bearing Arylphosphonic Acid Tethers for Attachment to Oxide Surfaces

AUTHOR(S): Muthukumaran, Kannan; Loewe, Robert S.; Ambrose, Arounaguiry; Tamaru, Shunichi; Li, Qiliang; Mathur, Guru; Bocian, David F.; Misra, Veena; Lindsey, Jonathan S.

CORPORATE SOURCE: Departments of Chemistry and Electrical and Computer Engineering, North Carolina State University, Raleigh, NC, 27695-8204, USA

SOURCE: Journal of Organic Chemistry (2004), 69(5), 1444-1452

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Synthetic mols. bearing phosphonic acid groups can be readily attached to oxide surfaces. As part of a program in mol.-based information storage, the authors have developed routes for the synthesis of diverse porphyrinic

compds. bearing phenylphosphonic acid tethers. The routes enable (1) incorporation of masked phosphonic acid groups in precursors for use in the rational synthesis of porphyrinic compds. and (2) derivatization of porphyrins with masked phosphonic acid groups. The precursors include dipyrromethanes, monoacyldipyrromethanes, and diacyldipyrromethanes. The tert-Bu group was used to mask the dihydroxyphosphoryl substituent. The di-tert-butyloxyporphoryl unit is stable to the range of conditions employed in syntheses of porphyrins and multiporphyrin arrays yet can be deprotected under mild conditions (TMS-Cl/TEA or TMS-Br/TEA in refluxing CHCl3) that do not cause demetalation of Zn or Mg porphyrins. The porphyrinic compds. that were prepared include (1) A3B-, trans-A3B2C-, and ABCD-porphyrins that bear a single phenylphosphonic acid group, (2) a trans-A2B2-porphyrin bearing two phenylphosphonic acid groups, (3) a chlorin that bears a single phenylphosphonic acid group, and (4) a porphyrin dyad bearing a single phenylphosphonic acid group. For selected

porphyrin-phosphonic acids, the electrochem. characteristics were studied for mols. tethered to SiO2 surfaces grown on doped Si. The voltammetric behavior indicates that the porphyrin-phosphonic acids form robust, elec. well-behaved monolayers on the oxide surface.

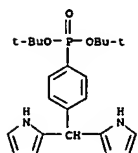
IT 651301-78-9P 651301-87-0P 651301-88-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reactant for preparation of zinc/magnesium complexes

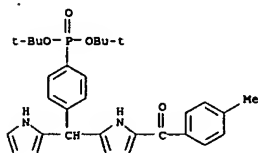
with porphyrins having arylphosphonic acid tethers)

RN 651301-78-9 CAPLUS

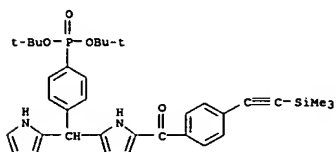
CN Phosphonic acid, [4-(di-1H-pyrrol-2-ylmethyl)phenyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



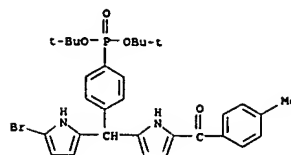
RN 651301-87-0 CAPLUS  
 CN Phosphonic acid, [4-[[5-(4-methylbenzoyl)-1H-pyrrol-2-yl]-1H-pyrrol-2-ylmethyl]phenyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



RN 651301-88-1 CAPLUS  
 CN Phosphonic acid,  
 [4-[1H-pyrrol-2-yl][5-[4-[(trimethylsilyl)ethynyl]benzoyl]-1H-pyrrol-2-yl]methyl]phenyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



IT 651302-30-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reactant for preparation of magnesium/zinc complexes with porphyrins having arylphosphonic acid tethers)  
 RN 651302-30-6 CAPLUS  
 CN Phosphonic acid, [4-[(5-bromo-1H-pyrrol-2-yl)[5-(4-methylbenzoyl)-1H-pyrrol-2-yl]methyl]phenyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

10.33

343.96

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-1.46

-2.92

STN INTERNATIONAL LOGOFF AT 15:33:14 ON 14 NOV 2005